

NREL Director's Discretionary Research and Development Program

**Annual Report
for Fiscal Year 2000**



NREL

National Renewable Energy Laboratory

1617 Cole Boulevard
Golden, Colorado 80401-3393

NREL is a U.S. Department of Energy Laboratory
Operated by Midwest Research Institute • Battelle • Bechtel

Contract No. DE-AC36-99-GO10337

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Executive Summary

Overview

Technical innovation is critical to the overall success of the National Renewable Energy Laboratory (NREL) and the U.S. Department of Energy (DOE) programs it supports. An important avenue for encouraging innovation at NREL is the Director's Discretionary Research and Development (DDRDR) program.

DOE's Office of Energy Efficiency and Renewable Energy (EE) established the DDRDR program in December 1998, and NREL implemented it in early 1999. DOE-EE's policy for the DDRDR program enables NREL's Director to

“...approve for funding projects put forth by laboratory staff which propose to explore and/or develop innovative or creative opportunities within mission areas assigned to the laboratory. Projects should advance research and development directed toward solving present scientific or technical problems; or should be experiments and analysis directed toward determining the merit and utility of new ideas or concepts.”

NREL's DDRDR program is similar to, but separate from, the Laboratory Directed Research and Development (LDRD) programs at other national laboratories. A significant distinction is that EE-NREL's program is specific to NREL as a single-program, renewable energy and energy efficiency research laboratory with technology deployment as part of its mission. NREL's mission, which is consistent with the DOE-EE mission, is

To lead the nation toward a sustainable energy future by developing renewable energy technologies, improving energy efficiency, advancing related science and engineering, and facilitating deployment.

The DDRDR program replaced previous laboratory-directed R&D programs at NREL originally called the Director's Discretionary or Development Fund (DDF) and later called Fostering Innovation, Research and Strategic Technologies (FIRST). Although the laboratory-directed R&D programs at NREL have changed to meet evolving strategic needs, each of these programs has been focused on advancing renewable energy and energy efficiency technologies, in support of the DOE-EE and NREL missions.

The objectives of NREL's DDRDR Program, as given in NREL's DDRDR policy, are to:

- Maintain the scientific and technical vitality of the Laboratory
- Enhance the Laboratory's long-term viability by strengthening core competencies and building new capabilities
- Enhance the Laboratory's ability to address future DOE missions
- Foster creativity and stimulate exploration at the forefront of science and technology
- Serve as a proving ground for new and potentially high-value mission enhancing activities.

By EE policy, the program may utilize up to 2% of the Laboratory's annual estimated funding from Appropriations, excluding funding specifically identified for capital equipment or for

construction. The specific level of funding is negotiated annually between NREL and the DOE Golden Field Office, in consultation with the EE Office of the Assistant Secretary. In fiscal year (FY) 2000, the approved ceiling was \$3 million. Individual projects can be authorized for funding up to \$500,000 for a period of performance up to three years, subject to annual funding authorization.

The DDRD program enables scientists to pursue cutting-edge science, thereby enhancing their scientific expertise and reputations and increasing their value as a resource to DOE and the nation. By being at the forefront of new scientific ideas, the scientists are able to attract new talent to the laboratory and maintain the vitality and viability of the scientific programs. As is the case with industrial leaders, the opportunity to pursue innovative ideas provides the foundation for advancement in technology and promotes creativity in the laboratory environment.

The 33 DDRD projects active in FY 2000 address a wide range of strategic research topics including bioenergy, biotechnology, chemistry, advanced materials for renewable energy technologies, advanced measurement and characterization techniques, distributed and hybrid energy systems, energy efficiency technologies, and energy analysis (Figure 1). These projects are intended to lay the groundwork for creating new or enhanced core competencies at NREL, to prove concepts to the point that they can attract future funding, or to enhance or expand NREL capabilities to carry out its mission.

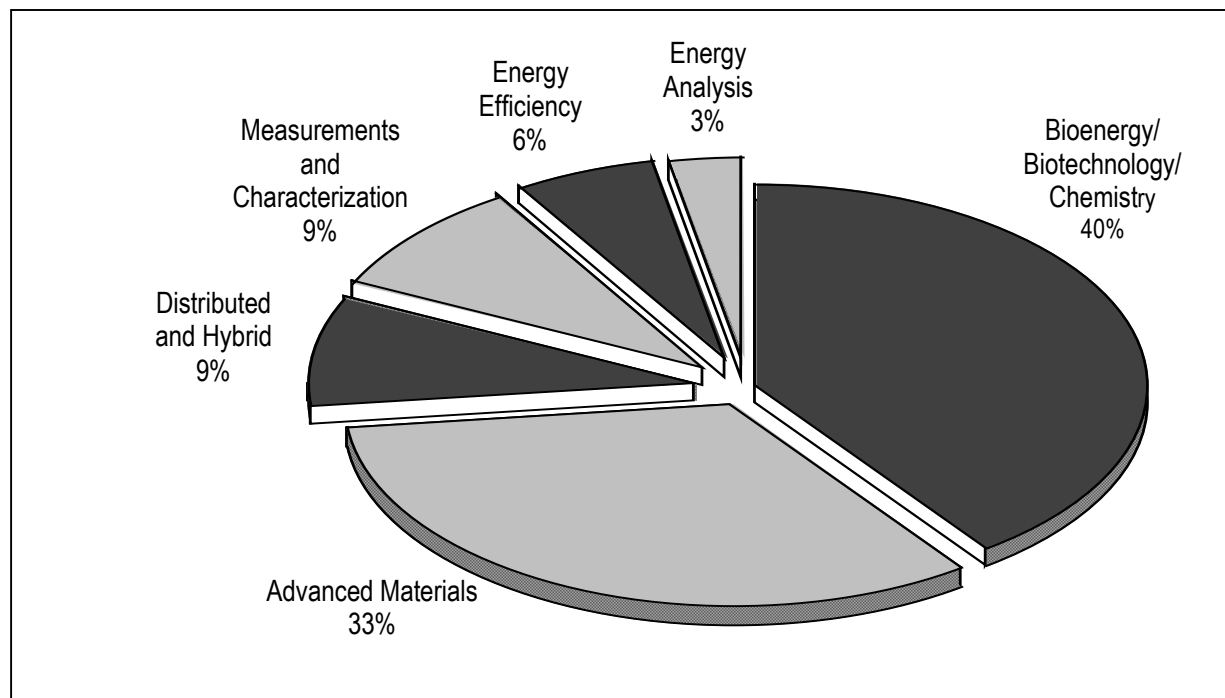


Figure 1. Allocation of DDRD projects by category. About half of the projects directly support distributed generation or bioenergy, two of NREL's strategic focus areas. Many of the other projects indirectly support these strategic areas.

This annual report lists funded and completed projects in FY 2000, describes each project and its outcomes, and summarizes the status and achievements of the DDRD program during FY 2000. The *Appendices* contain the NREL and DOE DDRD policies (Appendices A and B) and the DDRD Proposal Template (Appendix C).

DDRD Projects

In NREL's DDRD program, researchers are addressing the scientific topics described in Table 1, which underlie DOE's and NREL's missions and advance the strategies in NREL's 5-year plan.

Table 1. DDRD project scientific areas.

Bioenergy, Biotechnology, Chemistry	Page
Isolating genes responsible for carbon partitioning in plants to understand how to customize biomass for specific bioenergy purposes	16
Combining innovative chemical and biological techniques to screen natural plant variants for usefulness as biomass feedstock materials	17
Discovering genes in biomass (maize) that can be manipulated through genetic engineering to optimize the composition of biomass feedstocks for biomass conversion processes	19
Demonstrating a near-infrared spectroscopic technique to measure the properties of standing trees before they are cut down for selected uses	19
Examining the use of ionic liquids to convert biomass into useful chemicals without harmful emissions	20
Demonstrating that the two most abundant raw materials in nature – carbohydrates and lignin – can serve as important building blocks for conversion into polymers for commercial utility in a new biomass-to-chemicals industry	22
Developing the concept of biorefineries – complex processing strategies for efficiently producing a diverse and flexible mix of energy, fuel, chemical, and material products from lignocellulosic biomass resources	23
Exploring a special class of photosynthetic bacteria to produce biodegradable plastics	23
Creating a novel approach for developing electrocatalysts that increase the efficiency and decrease the costs of fuel cells	24
Advancing the fundamental understanding of photosynthesis to improve biomass production, algal hydrogen production, and artificial photosynthesis	24
Performing a proof-of-concept for a novel system for algal hydrogen production	25
Studying the role that organic radicals play in oxidizing hydrocarbons, whether in combustion of renewable fuels or in the environmental processing of pollutants in the atmosphere, using cryogenic spectroscopy techniques	25
Investigating the use of sunlight and photochemistry to convert biomass into high-density fuels	27
Advanced Materials for Renewable Energy Technologies	Page
Finding a simple, inexpensive, polycrystalline material for use in thermophotovoltaic – heat and electricity – power generation systems	28
Performing fundamental research on a new semiconductor material system for use as a thermophotovoltaic absorber	28

Table 1 (Cont'd). DDRD project scientific areas

Investigating low-temperature processes for purifying metallurgical-grade silicon to the degree necessary for solar-grade feedstock for photovoltaics	30
Advancing the fundamental understanding of limitations to polycrystalline solar cell efficiencies by optimizing the mechanism that lets light into the solar cell	30
Using combinatorial synthesis to discover new electronic materials thereby speeding up their discovery	31
Improving the conductivity of semiconductor layers which will in turn improve the efficiency of multi-layer photovoltaic devices	32
Pioneering an entirely new class of materials for application in microelectronics and photovoltaics industries	32
Applying a new materials synthesis approach to improve the performance of lithium batteries, electrochromic, and chemochromic devices which in turn will have a direct impact on the battery, electrochromic, and sensor industries	33
Developing fundamental understanding of dye-sensitized solar cells to improve their performance and expand the alternatives for solar energy conversion	33, 35
Developing new kinds of encapsulant materials that are convenient to handle and lead to a lower-cost encapsulation process for the photovoltaics industry	35
Advanced Measurement and Characterization Techniques	Page
Developing new spectroscopic techniques with time-resolved, sub-micron resolution to observe the optoelectronic properties of photovoltaic materials and thereby understand how to improve them	36
Strengthening the characterization methodology for thin-film photovoltaic materials to correlate the optical characteristics with the structural and electronic properties	38
Developing a surface-specific second-order nonlinear optical spectroscopy technique to understand photoelectrochemical, photocatalytic, electrocatalytic and charge-transfer reactions for renewable technologies	39
Distributed and Hybrid Energy Systems	Page
Advancing the basic science, design, development, and validation of the next generation of fuel cell systems	39
Exploring the feasibility of an integrated photovoltaic – solar concentrator as a next-generation technology to produce an inexpensive electric power system	40
Developing a new capability to estimate the hourly, multi-year solar resource for predicting performance and potential for deployment of renewable energy systems worldwide	40
Energy Efficiency Technologies	Page
Characterizing the performance of new airfoils that could significantly reduce the power requirements for cooling tower fans	41
Developing an advanced prototype of a component of refrigeration and air conditioning systems that will lower national energy consumption	42
Energy Analysis	Page
Testing the hypothesis that providing widely accessible, transparent, real-time energy analysis models will fundamentally advance the way renewable energy analysis is performed and communicated among energy analysts	42

Project Selection

NREL's executive management periodically issues calls for proposals from NREL staff, as funds are available. Proposals are submitted in a standard format using a proposal template (Appendix C). NREL's Research Fellows, led by the Senior Research Fellow, select teams of technical experts to review the proposals using a common set of evaluation criteria. With input from the review teams, the Research Fellows make recommendations to executive management on which proposals are technically sound. The Laboratory Director makes final selections of projects to fund under the DDRD program. Thirteen proposals were received following a call for DDRD proposals on June 1, 1999, and nine projects were approved for funding starting October 1, 1999 (FY 2000). In response to a call for DDRD proposals on February 1, 2000, twenty-one proposals were received, and six projects were approved for funding in May 2000. Including the 18 ongoing projects, this brought the number of active projects in FY 2000 to 33.

Measures of Success

Based on the NREL DDRD program goals specified in the policy, NREL's measures of success are:

- New or enhanced core competencies related to NREL's mission
- New hires that bring capabilities to the Laboratory and fill gaps in NREL's strategic staffing mix
- Enhanced scientific and technical vitality, including scientific recognition, papers, and awards
- Proof of concept picked up by current or new funding agencies in support of the DOE and NREL missions
- Scientific understanding that leads to go/no-go decision on path forward
- New or enhanced collaborations that enhance ability of the Laboratory to address future DOE missions
- Stimulated innovation as measured by
 - Diversity and quality of proposals
 - Laboratory participation in proposals and projects
 - Laboratory participation in DDRD presentations and seminars.

Together, the 33 projects active in FY 00 have thus far resulted in the following measures of success:

- 17 refereed articles
- 9 other papers
- 23 presentations
- 23 proposals
- 8 new sources of funding (for a total of \$2.2 million)
- 19 collaborations
- 2 new hires
- 3 records of invention

- 2 patents
- 1 major award

In addition to the new, cutting-edge science described in the Program Highlights below, the project descriptions starting on page 16 provide brief overviews and objectives as well as lists of publications, awards, intellectual property, presentations, collaborations, and follow-on research resulting from the DDRD funded-projects.

Program Highlights

Major advances in science and Laboratory capabilities have resulted from the individual projects within the DDRD Program in areas strategically important to the vitality and viability of the Laboratory and in support the NREL and DOE missions. Some of these advances and new capabilities are highlighted below.

Bioenergy / Biotechnology / Chemistry

- *Carbon Allocation and Partitioning in Woody Plants: A Means to Enhance Bioenergy Conversion and Carbon Sequestration.* In collaboration with researchers from the Oak Ridge National Laboratory, NREL scientists are attempting to determine the genetic basis for how carbon is allocated and partitioned into the cell walls of roots and stems of trees — a subject of utmost importance for carbon sequestration strategies and for thermochemical and biochemical conversion. Toward their goal, researchers have collected hybrid poplar wood and root samples, which they are analyzing to determine lignin, cellulose, and hemicellulose content.
- *Advancing Biotechnology R&D Capabilities at NREL.* With the intention of applying chemical techniques to solve biological problems, researchers in this project have successfully adapted the techniques of near infrared and pyrolysis molecular beam mass for use in screening biomass samples for characteristics important to biotechnology applications — a capability that holds great interest for industry – and have formed collaborations with industry and academic institutions. And they have been invited to join two projects of the National Science Foundation’s Plant Genome Initiative.
- *Prediction of the Mechanical Properties of Standing Trees.* Under this DDRD project researchers have developed a portable infrared spectroscopic technique for analyzing the mechanical properties of standing trees, such as wood stiffness and strength, density, and microfibril and grain angle. Armed with this information foresters can determine whether a tree would be best used for veneer, lumber, plywood, paper pulp, or should be left standing. R&D Magazine recognized this technology as one of the 100 most important new technologies for the year 2000.
- *Ionic Liquids as “Green” Reaction Media.* In this project, scientists have proven that ionic liquids — salt-like compounds that occur as liquids at room temperature — can be used to convert biomass-derived carbohydrates, such as glucose and xylose, into useful chemicals. In the process, they have learned how to prepare several types of ionic solvents on a routine basis, are developing a procedure that will allow us to isolate and purify products after completion of the chemical reactions, have discovered a new reaction that may be of great use in

lignin chemistry, and have created new opportunities to effect chemical reactions without the use of environmentally unfriendly acids such as sulfuric acid — a significant step towards the development of new “green chemistry.”

- *Photobiological Production of High-performance, Biodegradable Thermoplastics from Inexpensive Feedstocks by Photosynthetic Bacteria.* In their pursuit of photobiological production of high-performance, biodegradable thermoplastics from inexpensive feedstocks by photosynthetic bacteria, NREL researchers have successfully demonstrated the ability of several photosynthetic bacterial strains to operate in both light and dark. However, because the strains that produce well in the light are different from those that produce well in the dark, the researchers will continue to search for a single strain with high activities in both the light and dark, while considering a mixed-culture of bacteria to achieve the overall goal.
- *Development of Electrocatalysts Capable of Activating C-H and H-H Bonds.* Currently, fuel cells cannot use methane or other hydrocarbons directly, but must first reform them to hydrogen. This is inefficient. With this project, researchers are developing electrocatalysts that can oxidize C-H and H-H bonds and that can lead to the development of direct hydrocarbon fuel cells. To date they have synthesized new compounds containing transition metals with the desired structural features, which they will be testing for catalytic oxidation activity.
- *Comparative Study of the Interaction of Fe(II) and Mn(II) with the Manganese-binding Site of the Oxygenic Photosynthetic Apparatus.* In collaboration with two visiting Russian scientists, NREL researchers are well on their way toward a fundamental scientific understanding of photosynthesis processes, which will lead to improved biomass production, algal hydrogen production, and artificial photosynthetic processes.
- *Investigation of Organic Chemistry with Cryogenic Spectroscopy.* NREL researchers have developed a low-temperature photochemistry and spectroscopy technique that allows them to slow down the chemical reactions of organic radicals (which normally occur on the order of nanoseconds) and study the role that the radicals play in oxidizing hydrocarbons. This is a capability unique to NREL and is important for investigating fuel combustion and the environmental processes of pollutants in the atmosphere. The researchers have already used their technique to study the phenyl radical in detail and establish its basic electronic and vibrational spectroscopic signatures.
- *Photoconversion of Renewable Feedstocks for High Density Fuels and Energy Storage.* In this project, researchers are using sunlight and photochemistry to convert biomass into high-density fuels (hydrocarbons that have additional energy due to the presence of 3-, 4-, or 5-membered rings) for use in internal combustion engines. So far, researchers have synthesized and characterized target compounds and haven proven the concept that renewable feedstocks can be converted into high-density fuels.

Advanced Materials for Renewable Energy Technologies

- *Polycrystalline TPV Converters Based on Te-Se Alloys.* In an effort to design an advanced, inexpensive thermophotovoltaic cell, researchers investigated a promising polycrystalline material. Although their research showed that this material was inadequate for the proposed application, they were led to investigate an alternative material with better characteristics.
- *Low-Band-Gap GaInAsN Alloys for Advanced Thermophotovoltaic Energy Converters.* Thermophotovoltaic (TPV) devices can produce both electrical and thermal power from a single source. But TPV devices require a low-band-gap material such as promising alloys of

GaInAsN. In this project, researchers are studying these alloys to gain an understanding of the fundamental physics behind III-V nitrides. As a step toward their goal, researchers have first investigated the simpler alloy GaAs:N, and have published the results in *Physical Review B*.

- *Solar-grade Polysilicon Feedstock Development.* Researchers are studying the science underlying the potential development of solar-grade polysilicon feedstocks, which could prove crucial for the continued healthy growth of the silicon PV industry. In the course of their investigations they have discovered a unique, open-system chemical vapor transport process that has the potential to be used to purify silicon to the degree necessary to use for making solar cells.
- *Cadmium Tin Oxide Crystal Growth for Fundamental Studies.* To optimize thin-film transparent conducting oxides (which allow light into a thin-film cell and collect the current generated by it.) and thereby increase efficiencies of polycrystalline PV cells, researchers are growing single crystals of cadmium tin oxide and studying their fundamental characteristics. Toward this end, researchers have installed furnaces and control systems for growing the crystals via high-temperature solution and vapor sublimation. As a precursor toward their final goal, researchers have grown one of the component crystals — tin oxide.
- *Combinatorial Synthesis of Solid State Electronic Materials for Renewable Energy Applications.* NREL researchers have designed and developed two deposition systems and an analytical system that are needed to facilitate a combinatorial approach for discovering solid-state materials for renewable energy applications. They have also begun to create initial libraries with both deposition systems.
- *Reactive Codoping of Arsenide and Phosphide III-V Semiconductors for Improved Electrical Conductivity in Heavily Doped Layers.* Researchers are investigating novel co-doping concepts to improve the conductivity of window layers used on multijunction solar cells. This research could lead to a fundamental understanding that would enable us to make highly efficiency multijunction devices. Researchers have already grown, co-doped, and characterized several important materials; the results are highly encouraging.
- *Development of a New Class of Materials for Semiconductor Applications.* To broaden their scientific perspective on a new generation of silicon PV devices, NREL scientists are pioneering a new class of materials — microcrystalline silicon alloys — which may have application in the photovoltaic and microelectronics industries. To date, the scientists have deposited and characterized 50 microcrystalline silicon films.
- *The Characterization of Excited State Reactivity in Molecular Sensitizers.* Sensitizing photochemical solar cells with dyes makes the cells much more efficient. To gain a fundamental understanding of the dye sensitization process and to update theories of molecular photoconversion, NREL scientists explored the use of iron-based dyes in photochemical cells. They found that structural and environmental changes have an impact on the sensitization ability of the complexes in dye-sensitized solar cell devices. They also determined that iron sensitizers are viable alternatives to the more commonly used ruthenium-based analogues. Upon presenting these results to conferences and symposia, the researchers were invited to submit proposals to the Office of Basic Energy Sciences to obtain funding for basic research.
- *The Effect of the Orientation of the Excited State Dipole on the Efficiency and Polarity of Electron Transfer.* In this project researchers are investigating dye-sensitized photochemical solar cells to gain a fundamental understanding of the dye-sensitization process and to use this understanding to develop a new class of sensitizing dyes. Thus far, the researchers have

synthesized samples of a new class of sensitizing dyes. They have also found that the orientation of the excited state dipole affects the efficiency with which electrons are injected into the titanium dioxide of the photochemical cells — a finding that supports their hypothesis.

Advanced Measurement and Characterization Techniques

- *Time-resolved Spectroscopy of Photovoltaic Materials with Sub-micron Spatial Resolution.* Researchers developed an ultramodern technique for examining optoelectronic properties of PV materials on the nanoscale, and correlating those properties to the material's sub-micron topography. This gives NREL unique capabilities for characterizing PV materials and greatly enhances its leadership in this field.
- *Anisotropy in Hydrogenated Thin-film Silicon Material.* Researchers are optimizing new infrared spectroscopy techniques to gain novel insights into the structural and electronic properties of hydrogenated silicon thin-film materials. They have installed a new contact FTIR-ATR microprobe (a Fourier transform infrared spectroscope with an attenuated total reflection crystal) and used it to quantify the source of observed anisotropy in hydrogenated amorphous silicon. This new instrument extends NREL's capabilities in FTIR characterization.
- *Surface and Interface Studies by Second-order Nonlinear Optical Spectroscopy.* Surface reactions play a central role in photoelectrochemical, photocatalytic, and electrocatalytic reactions. Researchers are developing a spectroscopy technique to study the second-order, non-linear surface reactions. This technique could provide insight into the surface chemistry of fuel cell catalysis, dye-sensitization, and electron transfer, and may lead to improved designs for electrochemical and photoelectrochemical energy conversion devices. Currently, researchers are establishing the capability to acquire surface second harmonic generation data and fit the results to theory.

Distributed and Hybrid Energy Systems

- *Advanced Fuel Cells Research.* Researchers have built a test station and have used it to test commercial fuel-cell membranes. They have also established the ability to make cell membranes, which will boost fundamental research on fuel cells. And they have made substantial progress toward using ethanol directly in advanced fuel cells by enhancing and linking core competencies in fundamental theory of electrocatalysis and synthesis of advanced homogeneous catalysts — which has given them structural and electronic insights into ethanol oxidation rates and activation pathways.
- *Monolithically Integrated PV Modules for Dish Solar Concentrator Systems* Researchers have designed a small, high-efficiency PV cell with the structure and material properties that will enable it to operate appropriately under the spectrum and high flux levels of dish solar concentration. Once they have resolved the processing issues, they will monolithically connect the cells to produce a prototype module.
- *New Capabilities for Worldwide Weather Data Sets.* NREL researchers are merging rapid-data-access technology with their abilities to model solar radiation from weather records and to fill-in missing data. This will enable them to produce worldwide hourly input to computer programs that simulate the performance of a wide variety of renewable energy systems. This is a capability that users need to size and evaluate the performance and economics of systems being deployed worldwide.

Energy Efficiency

- *Performance Verification of NREL's Advanced Airfoils for Cooling Tower Fan Blades.* In a previous DDRD project, researchers used their expertise in wind turbine technology to design airfoils for cooling tower blades, with the expectation that the design would significantly reduce the power requirements for cooling tower fans. In this project they are verifying the performance of these advanced airfoils, and preliminary tests indicate that the design is exceeding expectations. The researchers are pursuing a patent, anticipating that the technology will be licensed to manufacturers.
- *Combined Compressor Pump Advanced Prototype.* This is a small (\$15K) DDRD project in which the researcher is building an advanced prototype to verify that his already successful design developed under the first phase of a DDRD project is economically feasible on small systems. Such a combined compressor pump will significantly lower the cost of energy-saving cooling designs and lead to lower energy consumption.

Energy Analysis

- *A Technology-Policy Expert System.* NREL analysts are changing the way energy analysis is conducted by establishing an internet-based capability that will allow analysts to collaborate on-line with remote colleagues and to evaluate the effectiveness of renewable energy policy. Already, the analysts have completed the system and application architectures and have merged financial and technology tools. They have also launched the Renewable Energy Analytic Studies Network to provide the basis for establishing a standard of practice in energy analysis.

Project Costs

Table 2 lists the FY 2000 project titles, principal investigators, total project award, the period of performance, pre-FY 2000 costs, FY 2000 costs, and post-FY 2000 estimated costs. FY 2000 costs are preliminary pending year-end fiscal-year costs close out.

Table 2. Project costs (in \$K) — actual and estimates

Project Title, Principal Investigator, Award, and Period of Performance	Pre 2000 Costs	FY 2000 Costs*	Outyear Estimate
Bioenergy, Biotechnology, Chemistry			
<i>Carbon Allocation and Partitioning in Woody Plants: A Means to Enhance Bioenergy Conversion and Carbon Sequestration</i> – Mark Davis; \$496K (\$150K in FY 2000); 10/99 – 9/02	0	115.0	381.0
<i>Advancing Biotechnology R&D Capability at NREL</i> – Steve Thomas; \$259.2K; 5/99 – 5/00 (completed)	133.8	146.5	0
<i>Functional Genomics of Transposon-Tagged Maize Cell Wall Biogenesis-Related Genes</i> – Steve Thomas; \$105.4K; 5/00 – 9/00 (expect to extend)	0	79.3	26.1

Table 2 (Cont'd). Project costs (in \$K) — actual and estimates

Project Title, Principal Investigator, Award, and Period of Performance	Pre 2000 Costs	FY 2000 Costs*	Outyear Estimate
<i>Prediction of the Mechanical Properties of Standing Trees</i> – Bob Meglen \$111.8K; 6/99 – 9/00 (no-cost ext. to 12/31)	18.6	84.4	8.8
<i>Ionic Liquids as “Green” Reaction Media</i> – Luc Moens \$169.3K; 3/99 – 2/01	38.3	118.0	13.0
<i>New Biobased Polymers and Chemicals from Carbohydrates and Lignin</i> – Joseph Bozell and Stephen Kelley; \$419.6K (\$75.6K in FY 2000); 7/00 – 6/02	0	17.4	402.2
<i>Realizing Biorefineries: Expanding the Sugars Platform Using New Biomass-Derived Sugar Products</i> – Jim McMillan, Rick Elander, and Kelly Ibsen; \$490K (\$32K in FY 2000); 7/00 – 6/03	0	18.9	471.1
<i>Photobiological Production of High-Performance, Biodegradable Thermoplastics from Inexpensive Feedstocks by Photosynthetic Bacteria</i> – Edward Wolfrum; \$96K (phase 1) 6/99 – 3/00 (extension date pending)	31	45.1	19.9
<i>Development of Electrocatalysts Capable of Activating C-H and H-H Bonds</i> – Daniel DuBois; \$190K; 6/99 – 5/01	17.6	70.5	101.9
<i>Comparative Study of the Interaction of Fe(II) and Mn(II) with the Manganese-Binding Site of the Oxygenic Photosynthetic Apparatus</i> – Michael Seibert; \$257.6K; 11/99 – 10/01	0	99.3	158.3
<i>Feasibility Studies for a Novel System for Algal Hydrogen Production</i> – Maria Ghirardi and William Jacoby; \$50K ; 10/99 – 9/00 (no-cost extension requested)	0	27.8	22.2
<i>Investigation of Organic Chemistry with Cryogenic Spectroscopy</i> – J. George Radziszewski; \$298.8K; 6/98 – 7/00 (completed)	215.7	96.1	0
<i>Photoconversion of Renewable Feedstocks for High-Density Fuels and Energy Storage</i> – Daniel Blake; \$179K; 4/98 – 9/00 (may extend)	122.8	40.5	15.7
Advanced Materials for Renewable Energy Technologies			
<i>Polycrystalline TPV Converters Based on Te-Se Alloys</i> – Kannan Ramanathan; \$200K; 7/98 – 9/00	91.2	67.2	0
<i>Low-Bandgap GaInAsN Alloys for Advanced Thermophotovoltaic Energy Converters</i> – Mark Wanlass and Angelo Mascarenhas; \$105K; 10/99 – 9/00 (may extend)	0	74.7	30.3
<i>Solar-Grade Polysilicon Feedstock Development</i> – Ted Cizek; \$313.4K; 5/99 – 4/01	84.1	143.9	85.4
<i>Cadmium Tin Oxide Crystal Growth for Fundamental Studies</i> – Ted Cizek; \$205K; 9/99 – 9/01	1.1	50.8	153.1
<i>Combinatorial Synthesis of Solid State Electronic Materials for Renewable Energy Applications</i> – David Ginley and John Perkins; \$100K; 10/99 – 9/00	0	124.1	62.0
<i>Reactive Codoping of Arsenide Phosphide III-V Semiconductors for Improved Electrical Conductivity in Heavily Doped Layers</i> – Mark Hanna; \$103K; 7/99 – 12/00	17.1	59.2	26.7

Table 2 (Cont'd). Project costs (in \$K) — actual and estimates.

Project Title, Principal Investigator, Award, and Period of Performance	Pre 2000 Costs	FY 2000 Costs*	Outyear Estimate
<i>Development of a New Class of Materials for Semiconductor Applications</i> – Harv Mahan; \$100K; 1/00 – 12/00	0	56.1	43.9
<i>Electrodeposited Mesoporous Transition Metal Oxides as Ion Insertion Hosts for Lithium Batteries, Electrochromics and Sensors</i> – John Turner; \$250K (\$33.2K in FY 2000); 6/00 – 5/02	0	29.6	220.4
<i>The Characterization of Excited State Reactivity in Molecular Sensitizers</i> – Suzanne Ferrere; \$212K; 4/98 – 5/00 (completed)	141.2	71.5	0
<i>The Effect of the Orientation of the Excited State Dipole on the Efficiency and Polarity of Electron Transfer</i> – Brian Gregg; \$246.6K; 10/99 – 9/01	0	102.0	144.6
<i>Development of New Encapsulants for Ambient (Non-Vacuum) PV Module Encapsulation</i> – John Pern; \$100K; (\$16.7K for FY 2000); 8/00 – 7/01 (waiting on post doc)	0	0	100.0
Advanced Measurement and Characterization Techniques			
<i>Time-Resolved Spectroscopy of Photovoltaic Materials with Sub-Micron Spatial Resolution</i> – Steve Smith and Angelo Mascarenhas; \$247K; 9/98 – 8/00	138.3	115.4	0
<i>Anisotropy in Hydrogenated Thin-Film Silicon Materials</i> – Brent Nelson; \$289.5K (\$100K for FY 2000); 10/99 – 9/01	16.1	81.4	208.1
<i>Surface and Interface Studies by Second-Order Nonlinear Optical Spectroscopy</i> – Randy Ellingson; \$300K; 10/99 – 9/02	0	100.5	199.5
Distributed and Hybrid Energy Systems			
<i>Advanced Fuel Cell Research</i> – John Turner; \$426K; 3/99 – 3/01	173.1	156.1	96.8
<i>Monolithically Integrated PV Modules for Dish Solar Concentrators</i> – Scott Ward; \$80K; 6/99 – 5/01	18.4	44.7	16.9
<i>New Capabilities for Worldwide Weather Data Sets</i> – Bill Marion; \$116.2K; 10/99 – 9/00	0	116.2	0
Energy Efficiency Technologies			
<i>Performance Verification of NREL's Advanced Airfoils for Cooling Tower Fan Blades</i> – James Tangler; \$78.2K; 7/99 – 9/00	9.6	68.6	0
<i>Combined Compressor Pump Advanced Prototype</i> – Christopher Gaul; \$15K (\$12.5K in FY 2000); 5/00 – 10/00	0	6.2	8.8
Energy Analysis			
<i>A Technology-Policy Expert System</i> – Sam Baldwin and Brandon Owens; \$500K; 10/98 – 9/01	147.3	194.5	158.2
Management and Close-out Costs on Previous DDRD Projects		19.9	
TOTALS		2641.4	3174.9
*Estimated pending year-end close out.			

Project Descriptions

In addition to project outcomes highlighted in the Executive Summary, this section provides a project description and objective for each project, as well as information on products and measures of success to date.

Bioenergy / Biotechnology / Chemistry

Mark Davis

Carbon Allocation and Partitioning in Woody Plants: A Means to Enhance Bioenergy Conversion and Carbon Sequestration

Award: \$496K (\$150K in FY 2000)

Period of Performance: 10/1/99 to 9/30/02

Project Number: 06570001

Status: In Process

Description: Designing or breeding biomass feedstocks with higher energy contents or feedstocks that are easily degraded is a central theme for the emerging renewable biomass-based industry. Conversely, producing biomass that is more resistant to degradation enhances the role of biomass in carbon sequestration/management strategies. The allocation and partitioning of fixed carbon can determine feedstock suitability for thermochemical and biochemical conversion, as well as the length of time carbon resides in soil. Thus, isolation of genes into complex developmental traits, and understanding the gene function would allow us to customize biomass for specific purposes.

This is a collaborative project with ORNL, which has funded parallel research projects through their LDRD program. Both NREL and ORNL have specific research tasks that will contribute to the overall success of the project.

Objective: The objective of this research is to characterize a genetic basis for understanding mechanisms controlling the quantity and quality of photosynthesis-derived carbon allocation into secondary cell walls of roots and stems of woody plants. That is, how many genes influence these traits? Where are they located in the genome? Do master regulatory (homeotic) genes exist for these traits?

Articles/Papers/Publications:

Refereed Journal Articles:

- Davis, Mark F.; Dinus, Ron; Tuskan, Gerald. "A Rapid Method for Measuring Syringyl to Guaiacyl Ratios in Hybrid Poplar." Article in preparation.

New or Enhanced Collaborations:

- A new collaboration has been developed with Tim Tschaplinski, who is leading the lignin precursor task at ORNL.
- Continuing collaboration with J. Tuskan (ORNL and LDRD Co P.I.).

Proposals / Follow-on Funding

Proposals

- A proposal (with ORNL taking the lead) is being submitted in response to DOE Office of Science Financial Assistance Program Notice LAB00-09: Carbon Sequestration Research Program. The new collaboration will broaden the scope of the research proposed in the original DDRD/LDRD effort to include leaf and fine root carbon allocation and partitioning.
- The collaboration with Tim Tschaplinski (above) has resulted in the proposal "Auxin Regulation of Wood Quality in Sweetgum and Loblolly Pine," (Tim Tschaplinski, ORNL, P.I.), submitted to OIT Agenda 2020 Forest Products call for FY 2001.
- The collaboration with J. Tuskan, above, (ORNL and DDRD/LDRD Co P.I.) has resulted in the proposal "Influence of Growth Environment and Silvicultural Practices on Wood Composition and Quality," (Davis, P.I., Tuskan and C. Nowak, SUNY, co-P.I.s), submitted to OIT Agenda 2020 Forest Products call for FY 2001.

Steven R. Thomas

Advancing Biotechnology R&D Capability at NREL

Award: \$259.2K

Period of Performance: 4/8/99 to 5/31/00

Project Number: 06580091

Status: Completed

Description: The strategic thrust of this project was to establish a strong plant biotechnology research and development capability to better position the Laboratory for its important role in bio-energy/biotechnology research and in development of national bioenergy initiatives. This project focused on development of reliable, high-throughput techniques that can be used to detect and quantify genetically determined chemical differences in plant biomass. The research crosscut two research centers at the Laboratory and built capability to address multiple technology goals.

Objective: The objective of this project was to apply chemical techniques to solve biological problems. Researchers used near-infrared (NIR) and pyrolysis molecular beam mass spectroscopy (pyMBMS) techniques to rapidly screen mutant plants for genetic variability in cell-wall chemistry. This screen will be a major tool in the eventual identification and isolation of genes involved in cell-wall biogenesis and structure (plant genomics). Such genes will eventually be useful in the optimization of biomass feedstock materials for biomass conversion processes. In addition, stover from varieties of corn known to have either altered lignin content or altered composition will be evaluated to determine whether or not altered chemical composition of stover translates into more easily convertible material, increased process yields, or decreased enzyme usage, any of which could result in an improvement in biomass conversion process economics. Our final objective was to establish a close working relationship with major players in plant biotechnology (industry, academia, and government).

Outcome. The project is complete, and we have accomplished all of our goals:

- In cooperation with an industrial collaborator, we have adapted NIR and pyMBMS techniques for use in screening dried maize leaf, stem, and grain samples.

- We identified unusual samples in the collection of 88 samples.
- We successfully screened over 5000 samples from a mutant collection of maize (provided by R. Martienssen and E. Vollbrecht of Cold Spring Harbor Lab — CSHL), and produced a statistical model for the population.
- We successfully established that NREL has capabilities of interest to the plant biotechnology community, formed collaborations with industry and academic labs, and been invited to join two different NSF Plant Genome Initiative projects.

In summary, this project demonstrated the utility of NIR and pyMBMS as useful genetic screening tools and identified genetic variants harboring tagged genes that will be useful in future genetic engineering approaches to tuning biomass composition for conversion processes.

Articles/Papers/Publications:

Refereed Journal Articles:

- Davis, Mark F.; Dinus, Ron; Tuskan, Gerald. "A Rapid Method for Measuring Syringyl to Guaiacyl Ratios in Hybrid Poplar." Article in preparation.

Presentations

- Thomas, S. "Identification of maize cell-wall mutations using near-IR spectroscopy: Implications for biomass to ethanol conversion." *American Chemical Society National Meeting*, March 26-30, 2000, San Francisco, CA (invited talk).
- Thomas, S. and R. Meglen "A Functional Genomics Approach to Cell Wall Biogenesis." *Plant Cell Wall Gordon Conference*, August 20-25, 2000, Meriden, NH (poster).

New or Enhanced Collaborations:

- A new collaboration has been developed Tim Tschaplinski, who is leading the lignin precursor task at ORNL.
- Continuing collaboration with J. Tuskan (ORNL and DDRD/LDRD Co P.I.).

Proposals / Follow-on Funding

Proposals

- A proposal (with ORNL taking the lead) is being submitted in response to DOE Office of Science Financial Assistance Program Notice LAB00-09: Carbon Sequestration Research Program. The new collaboration will broaden the scope of the research proposed in the original DDRD/LDRD effort to include leaf and fine root carbon allocation and partitioning.
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- The collaboration with J. Tuskan, above, (ORNL and DDRD/LDRD Co P.I.) has resulted in the proposal "Influence of Growth Environment and Silvicultural Practices on Wood Compo-

sition and Quality," (Davis, P.I., Tuskan and C. Nowak, SUNY, co-P.I.s), submitted to OIT Agenda 2020 Forest Products call for FY 2001.

Steven Thomas

Functional Genomics of Transposon*-Tagged Maize Cell Wall Biogenesis-Related Genes

Award: \$105,356 (tasks 1-3 of 9 tasks proposed); consideration of 4-9 in the future

Period of Performance: 5/1/00 to 9/30/00

Project Number: 06580001

Status: In Process

*A transposon is a genetic element (i.e., segment of DNA) that has the capability to move around in the genome to different locations, almost randomly. The insertion of a transposon into a gene typically inactivates that gene. Because the DNA sequence of the transposon is known, every mutation is "tagged" and it is relatively easy to clone DNA sequences around the insertion point.

Description: This project builds on a previous DDRD project that systematically laid the scientific and collaborative groundwork for a realistic and valuable plant biotechnology competency at NREL. Knowledge gained in the previous research regarding plant cell wall composition will be used to isolate and characterize genes that are involved in cell wall biogenesis, and eventually assist seed companies (i.e., the plant biotechnology industry) in breeding optimized feedstock materials for biomass conversion. This is the first time that plant biotechnology will be applied to the optimization of feedstock crops for bioenergy. This research is at the forefront of biomass conversion R&D, sophisticated analytical chemistry, chemometrics, and plant functional genomics.

Objective: The objective of this project is to discover genes in maize that can be manipulated through the use of genetic engineering to optimize the composition of biomass feedstocks for biomass conversion processes.

Robert Meglen

Prediction of the Mechanical Properties of Standing Trees

Award: \$45K (for phase I) \$66.8K (for phase II) total \$111.8K

Period of Performance: 6/99 to 9/00 (no-cost extension requested to 12/31/00)

Project Number: 06570093

Status: In Process

Description: Timber companies currently have limited knowledge of the quality of standing timber, which hinders their ability to anticipate the economic resource and to direct the various portions of the harvest to maximal use. NREL near-infrared (NIR) spectroscopy technology will allow them to drill a very small hole in the tree, insert an instrument probe, and know instantly key wood-quality parameters of the tree. Previous work provided chemical analysis capability to determine if the tree had enough cellulose for making paper. This project will add mechanical analysis capability to know if the wood will be strong and stiff enough to use for veneer or lumber.

Objective: The objectives of this research are to:

- Test the hypothesized relationship between the orientation of the cellulose chains and the differences in the chemical structure of lignin and wood mechanical properties by studying the fundamental relationships between the wood components and fiber anatomical characteristics using the NIR/PLS (projection to latent structure) techniques.
- Demonstrate the value of these NIR/PLS techniques for predicting the mechanical strength of standing timber in the field.

Awards

- 2000 R&D 100 Award (recognized by R&D Magazine as one of the 100 most significant new technologies of the year).

New or Enhanced Collaborations

- Collaborating with the United States Department of Agriculture, Southern Research Station, for field work.

Proposals / Follow-on Funding

Follow-on Funding

- Office of Industrial Technologies — \$647K
- Boise Cascade — \$18K
- U.S. Department of Agriculture, Southern Research Station — \$28K
- National Science Foundation (pending) — \$840K
- The researchers have also acquired DOE funding to support field testing of the methods on live trees. These tests will be performed in April / May 2000.

Intellectual Property (Patents, Records of Invention, etc.)

Records of Invention:

- Mechanical properties of standing timber using NIR

Luc Moens

Ionic Liquids as "Green" Reaction Media

Award: \$169.3K

Period of Performance: 3/1/99 to 2/28/01

Project Number: 06570084

Status: In Process

Description: Imagine organic solvents that save energy, are easily recycled, and do not generate the harmful air emissions of volatile organic compounds. Ionic liquids — a unique group of salt-like compounds that occur as liquids at room temperature — may fit the bill. In this project,

NREL researchers will use ionic liquids to convert biomass-derived carbohydrates, such as glucose and xylose, into useful chemicals. This will place NREL at the forefront of this exciting field, and not just for the biomass industry — NREL will be among the first groups in the United States to use ionic liquids for *any* organic synthesis.

Objective: The objective of this project is to research the use of ionic liquids for conversion of carbohydrates into useful chemicals.

Articles/Papers/Publications

Papers

- Moens, L. (Invited paper.) "Application of Room-Temperature Ionic Liquids (RTIL) to the Chemical Processing of Biomass-Derived Renewable Feedstocks". *NATO Advanced Research Workshop: Green Industrial Applications of Ionic Liquids*, April 12-16, 2000. Crete, Greece.

Presentations

- Moens, L. "Application of room-temperature ionic liquids to the chemical processing of biomass-derived renewable feedstocks." *American Chemical Society National Meeting*, March 26-30, 2000, San Francisco, CA.
- Moens, L. "Chemistry with carbohydrates and lignins in room-temperature ionic liquids." " *American Chemical Society National Meeting*, March 26-30, 2000, San Francisco, CA.
- Moens, L. (Invited presentation.) "Application of Room-Temperature Ionic Liquids (RTIL) to the Chemical Processing of Biomass-Derived Renewable Feedstocks". *NATO Advanced Research Workshop: Green Industrial Applications of Ionic Liquids*, April 12-16, 2000. Crete, Greece.
- Moens, L. Invited presentation on the state-of-the-art in the chemistry of ionic solvents. At Union Carbide in Charleston, WV, on May 9, 2000.
- Moens, L. Invited presentation on ionic liquids. *The DOE/OIT Industries of the Future Alabama Symposium*, July 26-28, 2000, Mobile, AL.

New or Enhanced Collaborations

- Collaboration begun with researchers of the Solar Thermal Program at NREL — to identify new types of ionic liquids that can be used in the parabolic trough technologies for solar heat storage.
- Strong informal working relationship with Professor Robin Rogers of the University of Alabama — R&D of ionic liquids for extraction technologies, with a focus on biomass-related analytical chemistry and extraction technologies.
- Informal working relationship with Professor Jim Davis of the University of South Alabama — who is doing research on synthetic chemistry using ionic solvents, and who will provide NREL with samples of new ionic liquids that will benefit the DDRD project.

- Agreement for future collaboration, under a DOE/OIT proposal, with the Fluorine Division of Ozark-Mahoning, a subsidiary of Elf Atochem North America, Inc. — to find an industrial partner who has an interest in using the ionic liquids for new commercial chemical processes.

Proposals / Follow-on Funding

Proposals

- Pre-proposal was sent to an EPA Green Chemistry Program in January, 2000. It focused on R&D dealing with oxidation chemistry in ionic liquids.
- Collaborated with Professor John Simonsen at the Oregon State University (Department of Forest Products) on a proposal to the USDA/NRI program — to devise a combinatorial approach towards catalyst development for new oxidation chemistry with lignin.
- Collaborated with Professor Robin Rogers (U. of Alabama), on a proposal to the Dreyfus Foundation — for R&D on ionic liquids chemistry.
- Preparing pre-proposals for NSF as a subcontractor to the group of Professor Jim Davis at the University of South Alabama. This is meant to be a continuation/expansion of the work on ionic liquids under the DDRD project.

Follow-on Funding

- USDA/NRI program (see proposal, above) — \$10,000

Joseph Bozell and Steve Kelley

New Biobased Polymers and Chemicals from Carbohydrates and Lignin

Award: \$419,570 (\$75,628 in FY 2000)

Period of Performance: 7/1/00 to 6/30/02

Project Number: 06570002

Status: In Process

Description: The existing chemical industry is heavily based on “platforms” — key intermediates that can fan out into dozens of other products. The compounds to be investigated in this work are superb platform candidates in the context of a biobased products industry. This research will investigate the conversion of these building blocks into polymers and evaluate their commercial utility as platforms in a new biomass-to-chemicals industry. NREL is teaming with researchers at the Pacific Northwest National Laboratory to combine catalysis and biochemical expertise (PNNL) with polymer and chemical expertise (NREL) to establish an overall core competency in polymer and chemical production from biomass, thereby positioning the Laboratories to respond effectively to the national biobased products and bioenergy initiatives.

Objective: The objective of this research is to demonstrate that the two most abundant raw materials in nature, carbohydrates and lignin, can serve as sources of important chemical building blocks, and to demonstrate new conversion technologies. The research is specifically directed at addressing a technology gap in the efficient use of renewables as chemical feedstocks; i.e., the lack of technological tools for the efficient conversion of renewables-based building blocks into products.

Jim McMillan, Rick Elander, and Kelly Ibsen

Realizing Biorefineries: Expanding the Sugars Platform Using New Biomass-Derived Sugar Products

Award: \$490K (\$31,995 in FY 2000)

Period of Performance: 7/1/00 to 6/30/03

Project Number: 06580002

Status: In Process

Description: In August 1999 President Clinton's issued Executive Order 13134, establishing the challenging goal of tripling the nation's production and use of bio-based products and bio-energy by 2010. According to the National Resources Council, the integrated biomass refinery, or "biorefinery", which would employ numerous conversion technologies to produce a variety of products from biomass in an integrated and flexible manner, represents one future vision of a bio-based products industry. This project advances NREL's knowledge and capabilities in developing biorefineries, i.e., complex processing strategies for efficiently producing a diverse and flexible mix of energy, fuel, chemical, and material products from renewable lignocellulosic biomass resources.

Objective: This project focuses strictly on identifying opportunities to use lignocellulosic biomass to expand the existing industrial sugars platform. The objective of this research is to establish NREL at the forefront of anticipating, investigating, reporting, and leading renewable energy and energy efficiency-driven changes in world sugar production and utilization patterns.

Edward Wolfrum

Photobiological Production of High-performance, Biodegradable Thermoplastics from Inexpensive Feedstocks by Photosynthetic Bacteria

Award: \$96K (to go/no-go decision point)

Period of Performance: 6/99 to TBD

Project Number: 06570092

Status: On hold (due to researcher illness) until Fall 2000

Description: Plastics are great — for many uses, too great. Use them once, throw them away, and they last forever as trash. With this project, NREL researchers have a better idea: use a special class of photosynthetic bacteria (already isolated by NREL scientists) to produce *biodegradable* plastics. These microbes feed on dilute organic waste streams, storing energy as biodegradable plastics — similar to how animals store fat. In the first phase of this project, researchers are manipulating growth conditions of the photosynthetic bacteria to control the yield and composition of the plastics. In a subsequent phase, researchers will develop a photoreactor for efficient, cost-effective production of the plastics.

Objective: The objectives of this research are to:

- Control the yield and chemical composition of the poly-3-hydroxyalkanoate (PHA) polymers by controlling the growth conditions of the photosynthetic bacteria

- Increase our understanding of the dynamics and efficiencies of photobioreactors for growth of microbial polymers.

Daniel DuBois

Development of Electrocatalysts Capable of Activating C-H and H-H Bonds

Award: \$190K

Period of Performance: 6/99 to 5/01

Project Number: 06590093

Status: In Process

Description: Fuel cells that could use hydrocarbons directly without having to reform them first would capture between 15% and 20% of the energy typically lost in the conversion of methane to methanol. With this project, researchers will develop electrocatalysts for breaking C-H and H-H bonds of hydrocarbons and hydrogen, respectively. Success could contribute to the feasibility of direct hydrocarbon fuel cells, and also improve the cost and energy efficiency of hydrogen fuel cells. The basic science related to C-H and H-H bond activation would also be advanced.

Objective: This objective of this research is to develop a novel approach for designing electrocatalysts that are capable of oxidizing C-H and H-H bonds.

New or Enhanced Collaborations

- Collaboration with Professor Mary Rakowski DuBois, University of Colorado (see Proposals/Follow-on Funding, below)

Proposals/Follow-on Funding

- A joint proposal with Professor Mary Rakowski DuBois, University of Colorado, was funded by the National Science Foundation (start date 3/1/00). This proposal was based on some of the underlying principles being developed here, but focuses on M-H bond strengths of Co, Rh, and Ir complexes.

Michael Seibert

Comparative Study of the Interaction of Fe(II) and Mn(II) with the Manganese-binding Site of the Oxygenic Photosynthetic Apparatus

Award: \$257.6K

Period of Performance: 11/1/99 to 10/31/02

Project Number: 06590092

Status: In Process

Description: Oxidation of water — a key part of the photosynthesis process that provides the Earth's oxygen — is not nearly as well understood at the molecular level as other aspects of photosynthesis. NREL scientists have developed strong expertise in isolating and examining the site of this reaction, a manganese-binding protein. Russian scientists have observed that this protein can also bind iron, probably at the manganese site. This project has initiated collaboration with the Russian team to study the differences resulting from substituting iron for manganese and

maybe unlock some of the secrets of photosynthesis in the process. The work could help improve biomass production, algal hydrogen production, and artificial photosynthetic processes.

Objective: The objective of this research is to advance scientific knowledge of photosynthesis by helping to define the assembly process and structural organization of the water-oxidizing system in the photosynthetic membranes of algae.

Maria Ghirardi and William Jacoby

Feasibility Studies on a Novel System for Algal Hydrogen Production

Award: \$50K for two phases

Period of Performance: 10/99 to 9/00 (no cost extension requested)

Project Number: 06590001

Status: In Process

Description: Using the hydrogenase enzyme to catalyze the photosynthetic algal production of hydrogen from water is a potentially efficient source of clean, renewable energy. However, practical implementation of this system has been hampered in the past due to the extreme sensitivity of the hydrogenase enzyme to oxygen, one of the byproducts of photosynthesis. In this project, researchers will complete an initial assessment of the potential of a novel algal H₂-production system that overcomes these barriers to commercial production.

Objective: The objective of this research is to design, fabricate, and operate an innovative photobioreactor to study the technical and economic feasibility of using a novel H₂-producing system as a commercial process for producing renewable energy.

J. George Radziszewski

Investigation of Organic Chemistry with Cryogenic Spectroscopy

Award: \$298.8K

Period of Performance: 6/1/98 to 7/31/00

Project Number: 06570082

Status: Completed

Description: It would certainly seem easier to understand a key chemical reaction if it took days to occur instead of its natural nanoseconds. Effectively, that is what researchers did with this project. They used near absolute zero temperatures to slow down reactions and isolate otherwise extremely short-lived organic radicals (hydrocarbon molecules with a hydrogen atom stripped off) that occur as a result of hydrocarbon combustion. This enabled them to use refined optical spectroscopy to “fingerprint” the radicals. They have already published a paper conclusively showing success in fingerprinting radicals — something that has not been achieved in 30 years of attempts by others.

Objective: The objective of this research was to study the role that organic radicals play in oxidizing hydrocarbons, whether in combustion of renewable fuels or in the environmental processing of pollutants in the atmosphere, using cryogenic spectroscopy techniques.

Outcome: The research has two direct benefits to businesses involved in combustion and atmospheric chemistry: (1) it leads to a detailed understanding of important chemistry in these processes, and (2) it provides spectroscopic signatures for analytical chemists dealing with these important radical intermediates.

For NREL, the research led to new spectroscopic analytical techniques, establishing NREL's leadership in this important area of basic science. It will also led to a better understanding of combustion of renewable fuels; this could help us increase combustion efficiencies and mitigate the emission of pollutants. In addition, specific results were:

- We have created a low-temperature photochemistry and spectroscopy laboratory capable of studying basic bioenergy problems. This laboratory has several unique, fully operational instrumental set-ups that enhance NREL's experimental capabilities.
- We have studied the phenyl radical (the simplest of the large family of aromatic radicals) in detail, and have established basic electronic and vibrational spectroscopic signatures for this first model compound.
- We worked on several other important radicals (phenyl peroxy, phenoxy).

Articles/Papers/Publications

Refereed Articles

- Radziszewski, G.J. "Electronic absorption spectrum of phenyl radical." *Chem. Phys. Let.*; Vol. 301, 1999, pp. 565-570.
- Rowland, B; Winter, P.R, Ellison, B.; Radziszewski, J.G.; Hess, W.P. "Photochemistry of Matrix Isolated and Thin Film Acid Chlorides: Quantum Yields and Product Structures." *J. Phys. Chem A* 1999, Vol. 103, pp. 965-970.

Papers

- Radziszewski, J.G. "Aromatic Radicals in Combustion." Submitted paper.

Presentations

- Radziszewski, J.G. "High Energy Density Materials." *AFOSR Conference*, Cocoa Beach, FL, June 1999.
- Radziszewski, J.G. Invited Lecture. Department of Chemical Engineering and Petroleum Refining, Colorado School of Mines, November 1999.

Proposals / Follow-on Funding

Proposals

- Proposal: *Aromatic Radical in Biomass Gasification*. Submitted to the DOE Office of Basic Sciences.

- Proposal: *Instrumentation for Simultaneous Multi-technique (IR, Raman, UV, Luminescence) Spectral Studies of Highly Reactive Intermediates Relevant in Combustion and Deflagration Problems*. Submitted to the Chemistry Research Instrumentation and Facility Program of the National Science Foundation.
- Proposal: *Spectroscopy and Chemistry of Aromatic Radicals Relevant in Combustion*. Submitted to The Petroleum Research Fund American Chemical Society (resubmitted 1/28/00).
- Proposal: *Spectroscopy and Chemistry of Organic Radicals Relevant in Combustion*. Submitted to NATO Science Program.

Follow-on-Funding

- Funding from the Chemistry Research Instrumentation and Facility Program of the National Science Foundation. For proposal to same (see above), for collaboration with the Colorado School of Mines. Funding: \$180K government funds, \$75K CSM matching, \$140K other CSM funds.

Daniel Blake

Photoconversion of Renewable Feedstocks for High Density Fuels and Energy Storage

Award: \$179K

Period of Performance: 4/1/98 to 9/30/00 (may extend)

Project Number: 06430078

Status: In Process

Description: In this project, researchers are using sunlight and photochemistry to convert biomass into high-density fuels for use in internal combustion engines. High-density fuels are hydrocarbons that have additional energy due to the presence of 3-, 4-, or 5-membered rings. The formation of rings employing photochemistry may also be used to soak up and store sunlight energy. Success would position NREL at the forefront of this novel area of research and build NREL's capabilities in organic synthesis and photochemistry that can be applied in the Bio-energy initiative.

Objective: The objective of this research is to investigate the photoconversion of renewable feedstocks into high-density fuels.

Advanced Materials for Renewable Energy Technologies

Kannan Ramanathan

Polycrystalline TPV Converters Based on Te-Se Alloys

Award: \$200K

Period of Performance: 7/1/98 to 9/30/00

Project Number: 06520081

Status: In Process

Description: NREL has helped pioneer the technology for making low-band-gap thermophotovoltaic (TPV) cells that convert infrared light, such as that generated by the heat of engines, into electricity. But the cells are expensive, single-crystal cells made with III-V materials, with a market limited to those who can afford them (such as the military). Researchers in this project are developing the ability to make inexpensive, low-band-gap polycrystalline cells that could expand the TPV markets and that could be used as a bottom cell in a polycrystalline tandem device.

Objective: The purpose of this research is to find a simple, inexpensive, polycrystalline material for use in TPV systems, which convert infrared light, such as that generated by the heat of engines, into electricity.

Intellectual Property (Patents, Records of Invention, etc.)

Records of Invention

- Rammanathan, K. "Te-Se Alloy-Based TPV Devices," NREL Record of Invention IR#98-41.

Angelo Mascarenhas and Mark Wanlass

Low-Band-Gap GaInAsN Alloys for Advanced Thermophotovoltaic Energy Converters

Award: \$105K

Period of Performance: 10/1/99 to 9/30/00 (may extend)

Project Number: 06520002

Status: In Process

Description: One of NREL's strategic thrusts, distributed and hybrid generation, is focused on development and deployment of systems that produce both electrical and thermal power from a single source. The characteristics of thermophotovoltaic (TPV) power generation systems address the objectives of this strategic area. NREL is a pioneer in the area of TPV, and this project will build on the existing experimental and theoretical knowledge base on Nitrides developed at NREL. The goal is to develop an improved materials approach for TPV converter fabrication, thus improving the efficiency of the TPV process and enhancing the likelihood of TPV system deployment. The proposed materials concepts involve advanced GaInAsN alloys. An investigation of these alloys could lead to advanced understanding of the fundamental physics related to the alloys.

Objective: The objective of this research is to address the technological challenge of obtaining a good 0.5 eV band gap semiconductor for use as a TPV absorber. This will be done by performing fundamental research on GaInAsN and GaAsSbN systems, which are potentially excellent choices for this system.

Articles/Papers/Publications

Refereed Journal Articles

- Zhang, Y.; Mascarenhas, A.; Xin, H.P.; Tu, C.W. "Valence-band splitting and shear deformation potential of dilute GaAs_{1-x}N_x alloys." *Phys. Rev B* **61**, 4433 (2000).
- Zhang, Y.; Mascarenhas, A.; Xin, H.P.; Tu, C.W. "Formation of an impurity band and its quantum confinement in heavily doped GaAs:N." *Phys. Rev B* **61**, 7479 (2000).
- Zhang, Y.; Ge, W.K. "Behavior of Nitrogen Impurities in III-V Semiconductors." *J. Lumin.* **85**, 247 (2000).
- Zhang, Y.; Mascarenhas, A.; Xin, H.p.; Tu, C.W. "Valence-band splitting and shear deformation potential of dilute GaAs_{1-x}N_x alloys." *Phys. Rev. B* **61**, 4433 (2000).
- Zhang, Y.; Mascarenhas, A.; Xin, H.p.; Tu, C.W. "Formation of an impurity band and its quantum confinement in heavily doped GaAs:N." *Phys. Rev. B* **61**, 7479 (2000).
- Zhang, Y.; Mascarenhas, A.; Xin, H.p.; Tu, C.W. "Effects of nitrogen on the band structure of GaN_xP_{1-x} alloys." *Appl. Phys. Lett.* **76**, 1267 (2000).
- Kozhevnikov, M.; Narayanamurti, V.; Reddy, C.V.; Xin, H.P.; Tu, C.W.; Mascarenhas, A.; Zhang, Y. "Evolution of GaAs_{1-x}N_x conduction states and giant Au/GaAs_{1-x}N_x Schottky barrier reduction studied by ballistic electron emission microscopy." *Phys. Rev. B* **61**, R7861 (2000).
- Cheong, H.M.; Zhang, Y.; Mascarenhas, A.; Geisz, J.F. "Observation of nitrogen-induced levels in GaAs_{1-x}N_x using resonant Raman studies." *Phys. Rev. B* **61**, 13687 (2000).
- Zhang, Y.; Mascarenhas, A. "Isoelectronic impurity states in GaAs:N." *Phys. Rev. B* **61**, 15562 (2000).
- Zhang, Y.; Fluegel, B.; Mascarenhas, A.; Xin, H.P.; Tu, C.W. "Optical transitions in isoelectronically doped semiconductor GaP:N: an evolution from isolated centers, pairs, clusters to an impurity band." *Phys. Rev. B* **62** (August, 2000).

Presentations

- Results were presented at the American Physical Society's March 2000 meeting in Minneapolis.

New or Enhanced Collaborations

- Collaborating with Harvard University and Iowa State University on this project.

Ted Ciszek

Solar-grade Polysilicon Feedstock Development

Award: \$313.4K

Period of Performance: 5/1/99 to 4/30/2001

Project Number: 06590091

Status: In Process

Description: To keep growing at a healthy pace, the crystalline silicon PV industry needs an inexpensive, dependable supply of solar-grade silicon. In this project, researchers are exploring two innovative, low-temperature, low-cost methods for purifying metallurgical-grade silicon to the degree necessary to be able to use it as solar-grade feedstock. Any successful process resulting from this project would likely be quickly adapted by the industry.

Objective: The objective of this research is to investigate two low-temperature processes for purifying metallurgical-grade silicon to the degree necessary for solar-grade feedstock.

Intellectual Property (patents, records of invention, etc.)

Patents

- A provisional patent application has been filed on the recrystallization from metal solution approaches. Based on this patent application, a non-disclosure agreement has been written and is to be put in place with GT Equipment Technology Corp.

Records of Invention

- A record of invention is currently being written for the iodine vapor transport purification approach.

Ted Ciszek

Cadmium Tin Oxide Crystal Growth for Fundamental Studies

Award: \$205K

Period of Performance: 9/99 to 9/01

Project Number: 06590094

Status: In Process

Description: How high can we push conversion efficiencies of thin-film polycrystalline PV cells? Part of the answer lies in how well we can optimize thin-film transparent conducting oxides, or TCOs (which allow light into a thin-film cell and collect the current generated by it.) This project is exploring such an optimization by fabricating and characterizing a single-crystal version of an important TCO material — cadmium tin oxide. Success in this project will enable NREL to make better thin-film TCOs and to increase efficiencies of polycrystalline materials toward their optimum.

Objective: The objective of this research is to grow and characterize single crystals of Cd_2SnO_4 , which is used in a thin film form as a transparent conducting oxide. Characterizing single crystal Cd_2SnO_4 should lead to a better understanding of the thin-film version and help remove its limitations as a TCO.

David Ginley and John Perkins

Combinatorial Synthesis of Solid State Electronic Materials for Renewable Energy Applications

Award: \$100K (up to \$350K when reassessed at the \$100K mark)

Period of Performance: 12 months from 10/1/99 to \$100K mark

Project Number: 06520001

Status: In Process

Description: Currently, there is very little work underway to discover new materials suitable for application as absorber layers for areas such as photovoltaics, as transparent conductors, and as intercalation materials for lithium batteries. In each case, work tends to continue on the development and refinement of existing materials for these applications. However, recent work has shown that in many of these areas there are large areas of synthesis phase space that may be profitably explored for new materials. The problem is that by proceeding in a linear compound-by-compound fashion, discovery is slow and synergistic interactions between elements are often missed. The NREL researchers propose a novel combinatorial approach aimed specifically toward solid-state electronic materials for renewable energy applications.

Objective: The objective of this research is to develop a solid-state combinatorial capability for the synthesis and discovery of new electronic materials as well as for the optimization of existing materials.

Presentations

- Wang, Q. "Materials Transition from a-Si:H to $\mu\text{c-Si}$ Deposited by Combi-HWCVD." *Materials Research Society Symposium on Combinatorial Chemistry and Materials Science*, Spring 2000.

New hires with capabilities that fill gaps in NREL's strategic staffing mix

- We and Professor Dennis Readey have mutually obtained the services of Colorado School of Mines graduate student Chris Duncan, who will be doing his graduate thesis work with our group at NREL. Towards this end, a new task order has been established with Prof. Dennis Readey at CSM to support this work. To date, Chris has only been able to work part time on this project due to both classes and teaching responsibilities at CSM. After this term he will work full-time with us on this research project.

New or Enhanced Collaborations

- Collaboration interaction with Professor Dennis Readey of the Metallurgy/Ceramics Department of the Colorado School of Mines (see above).

Proposals / Follow-on Funding

- Proposals have been submitted to BES Materials and Chemical Sciences.

Mark Hanna

Reactive Codoping of Arsenide and Phosphide III-V Semiconductors for Improved Electrical Conductivity in Heavily Doped Layers

Award: \$103K

Period of Performance: 7/99 to 12/00

Project Number: 06590095

Status: In Process

Description: NREL research is on the verge of making very high efficiency (approaching 40%) 3- and 4-junction cells from III-V materials. One of the problems is that normal doping techniques for the AlInP window layer used on such cells result in insufficient conductivity, which limits the efficiency of the entire device. Success in this project will not only produce a highly conductive window layer for 3- and 4-junction cells, it will also give us a doping approach that will increase the efficiency of 2-junction cells, especially under concentrated sunlight.

Objective: The objective of this research is to improve the conductivity of heavily doped III-V semiconductor layers and thus improve the efficiency of III-V multijunction devices.

Harv Mahan

Development of a New Class of Materials for Semiconductor Applications

Award: \$100K

Period of Performance: 1/00 to 12/00

Project Number: 06520002

Status: In Process

Description: In this project, researchers will pioneer a new class of materials — microcrystalline silicon alloys — for application in the microelectronics and photovoltaics industries. Because of extensive experience and knowledge, the amorphous silicon team at NREL is uniquely poised to develop these materials. Through interaction with the microelectronics-photonics community in this project, NREL scientists will broaden their scientific perspective regarding the next generation of microcrystalline-silicon-based PV devices.

Objective: The objective of this research is to investigate a new class of materials with potential application to the microelectronics and photovoltaic industries.

John Turner

Electrodeposited Mesoporous Transition Metal Oxides as Ion Insertion Hosts for Lithium Batteries, Electrochromics and Sensors

Award: \$250K (\$31,110 in FY 2000)

Period of Performance: 6/1/00 to 5/31/02

Project Number: 06590005

Status: In Process

Description: In the past two decades, research on ion-insertion metal oxides has established that one of the limitations for lithium batteries and electrochromic devices is governed by the diffusion of Li⁺ or H⁺ in the oxide framework. Employing a highly porous material is one of the strategies used to reduce the length of the diffusion path and increase the performance. This research is directed at solving the dilemma of performance versus manufacturability. High-performance materials are often difficult and expensive to manufacture. The synthesis approach proposed in this research should provide high-performance materials that can be inexpensively manufactured.

Objective: The objective of this research is to apply a new materials synthesis approach developed at NREL to metal oxides that are of great interest to industry in improving the performance of lithium batteries, electrochromic, and chemochromic devices. This, in turn, will have a direct impact on the battery, electrochromic, and sensor industries.

Suzanne Ferrere

The Characterization of Excited State Reactivity in Molecular Sensitizers

Award: \$212K

Period of Performance: 5/4/98 to 5/3/00

Project Number: 06590082

Status: Completed

Description: NREL has successfully combined dye-sensitized photochemical solar cell (Graetzel cell) technology into other technologies such as that for self-powered photoelectrochromic windows. U.S. expertise in photochemical solar cells themselves, however, is limited. This project explored the use of iron-based rather than ruthenium-based dyes — initial work indicates great promise — and builds on the work NREL has done with photochemical solar cells to help establish NREL as the U.S. leader in the field.

Objective: The objective of this research was to determine and characterize the parameters of the sensitizing dye that control excited state reactivity and charge injection in dye sensitized solar cells. The goals were to gain a better understanding of the dye sensitization process, update theories of molecular photoconversion, and establish a foundation to obtain basic research funding.

Outcome: We have completed all of the work planned with the iron bipyridyl systems. We found that structural changes and environmental changes do have an impact on the sensitization ability of the complexes in the dye-sensitized solar cell device. It is now necessary to do time-resolved spectroscopy on the system to fully understand the effects.

We have presented our results to conferences, symposia, and program reviews. As a result of the exposure, we prepared an invited proposal to the Office of Basic Energy Sciences.

Articles/Papers/Publications

- Ferrere, S. "New Photosensitizers Based upon $[\text{Fe}(\text{L})_2(\text{CN})_2]$ and $[\text{Fe}(\text{L})_3]$ (L = Substituted 2,2'-Bipyridine): Yields for the Photosensitization of TiO_2 and Effects on Band Selectivity." *Chemistry of Materials*, Vol. 12, No. 4, pp. 1083-1089.
- Ferrere, S. "New Photosensitizers Based Upon $[\text{Fe}(\text{L})_2(\text{CN})_2]$ and $[\text{Fe}(\text{L})_3]$ Where L is Substituted 2,2'-Bipyridine: Synthesis, Spectral Characteristics and Electrochemical Behavior of the Complexes in Solution." Manuscript in preparation.

Presentations

- Ferrere, S. Invited speaker. "Dye Sensitization with Iron(II) Bipyridyl Complexes." 2000 Gordon Conference on Electrochemistry, Ventura, CA, January 2000.
- Ferrere, S.; Gregg, B.A. Poster. "Iron (II) Bipyridyl Complexes as Photosensitizers." 13th International Symposium on Photochemistry and Photophysics of Coordination Compounds, Lipari, Italy; June 1999.
- Ferrere, S.; Gregg, B.A. Poster. "Iron (II) Bipyridyl Complexes as Photosensitizing Dyes." DOE Solar Photochemistry Research Conference, Lake Tahoe, CA; June 1999.
- Ferrere, S. Invited speaker. 7th International SPACC (Society of Pure and Applied Coordination Chemistry) Symposium ñ Chemistry for Nano-scale Composite Systems, Osaka, Japan, July 2000.

New Hires with Capabilities that Fill Gaps in NREL'S Strategic Staffing Mix

- Suzanne Ferrere was hired as a regular employee (formerly temporary employee) in December 1999 in a Senior Scientist I position.

New or Enhanced Collaborations

- Collaboration with Professor Paul Rillema of Wichita State University, a ruthenium synthetic chemist.
- Collaboration with Dr. Shogo Nakade of Nokia Japan.

Proposals / Follow-on Funding

- At the invitation of Dr. Mary Gress, the proposal "Photoinduced Electron Transfer from Non-Equilibrated Excited States of Molecules Adsorbed to Nanocrystalline Semiconductors: Towards a Greater Fundamental Understanding of Upper Excited State Reactivity", was submitted to the photochemical sciences part of the Office of Basic Energy Sciences.
- Another proposal based on this work will be submitted to the National Nanotechnology Initiative call for proposal when announced.

Brian Gregg

The Effect of the Orientation of the Excited State Dipole on the Efficiency and Polarity of Electron Transfer

Award: \$246.6K (\$100K for FY 2000)

Period of Performance: 10/99 to 12/01

Project Number: 06590002

Status: In Process

Description: Dye sensitization has emerged as an unexpected alternative to conventional methods of converting solar energy. The best dye-sensitized solar cells now reach an efficiency of around 10% and cost potentially much less than silicon or thin-film solar cells. Although we are beginning to understand dye cells, there are still a number of open questions. This research is aimed at developing a new understanding of fundamental aspects of dye-sensitization and at developing a new set of sensitizing dyes. If successful, a number of scientific groups will begin the more detailed characterization of these systems and the elaboration of these ideas into improved versions of the dye cell.

Objective: The objectives of this research are to: (1) determine if the orientation of the excited state dipole effects the efficiency and polarity of electron transfer, (2) introduce a new class of sensitizing dyes with increased chemical stability and greater oscillator strength, (3) provide the first clear design criteria for hole-injecting dyes, and (4) provide the fundamental knowledge necessary to design a tandem dye-sensitized solar cell.

New or Enhanced Collaborations

Collaborating with Professor Clark Fields of the University of Northern Colorado on the synthesis of p-type semiconductors for the project.

John Pern

Development of New Encapsulants for Ambient (Non-Vacuum) PV Module Encapsulation

Award: \$100K (\$16,665 for FY 2000) (1-year of a 2-year proposal funded)

Period of Performance: 8/1/00 – 7/31/01

Project Number: 0650004

Status: Approved 5/2/00; delayed while finding post doc

Description: This research is designed to address head-on a critical bottleneck in a photovoltaic manufacturing process that is manifested by a labor-intensive vacuum-lamination encapsulation method using ethylene vinyl acetate (EVA). The researchers are developing new kinds of encapsulant materials that can be extruded into films or sheets that are convenient to handle and suitable for ambient (non-vacuum) lamination and encapsulation of crystalline silicon and thin-film PV modules. The combination of a non-vacuum ambient encapsulant with a heated-press lamination/encapsulation process would enable a substantial reduction in labor requirements, energy consumption, and cost of encapsulation equipment. It could also lead to process automation, resulting in a large increase in production speed and yield. With higher performance, more durable

encapsulants, and a lower cost encapsulation process, the U.S. PV industry will be in an advantageous position in global competition.

Objective: The objective of this research is to develop new kinds of encapsulant materials with formulations that can be extruded into films or sheets, that are convenient to handle, and that are suitable for ambient (non vacuum) lamination and encapsulation of crystalline silicon and thin-film PV modules.

Advanced Measurement and Characterization Techniques

Steve Smith and Angelo Mascarenhas

Time-resolved Spectroscopy of Photovoltaic Materials with Sub-micron Spatial Resolution

Award: \$247K

Period of Performance: 9/1/98 to 8/30/00

Project Number: 06520082

Status: In Process

Description: In the important emerging class of polycrystalline PV materials, chemical composition, doping, and optoelectronic properties vary from grain to grain. With this project, researchers are combining ultrafast spectroscopy with near-field scanning optical microscopy to develop an ultramodern technique for examining optoelectronic properties on the nanoscale, and correlating those properties to the material's sub-micron topography. This gives NREL unique capabilities for characterizing PV materials and greatly enhances its leadership in this field.

Objective: The objective of this research is to combine microspectroscopy techniques with NREL's state-of-the-art ultrafast spectroscopy capabilities to perform high spatial and temporal resolution studies of thin-film photovoltaic materials.

Articles/Papers/Publications

Refereed Journal Articles

- Smith, S.; Cheong, H.M.; Fluegel, B.D.; Geisz, J.F.; Olson, J.M.; Kazmerski, L.L.; Mascarenhas, A. "Spatially resolved photoluminescence in partially ordered GaInP₂," *Applied Physics Letters* 74 (5) 1 February 1999.
- Zhang, Y.; Mascarenhas, A.; Smith, S.; Geisz, J.F.; Olson, J.M.; Hanna, M. "Effects of spontaneous ordering and alloy statistical fluctuations in Ga_xIn_{1-x}P alloys," *Physical Review B*, 61 (15) 15 April 2000.

Other Papers

- Smith, S.; Cheong, H.M.; Fluegel, B.D.; Geisz, J.F.; Olson, J.M.; Kazmerski, L.L.; Mascarenhas, A. "Excitons and Recombination in Photovoltaic Materials," *AIP Conf. Proc.*, NCPV Program Review, Denver, CO, Sept. 1998.
- Smith, S.; Cheong, H.M.; Fluegel, B.D.; Geisz, J.F.; Olson, J.M.; Kazmerski, L.L.; Mascarenhas, A. "Spatially-resolved low-temperature photoluminescence in GaInP₂," *Quantum Optoelectronics: technical digest*, paper number QMD2-1, pg. 43, Aspen, CO, April 1999.
- Kao, Y.H.; Kazmerski, L.; Lynn, K.G.; Mascarenhas, A. "Photovoltaics characterization: An Overview", in *Photovoltaics for the 21st Century, The Electrochemical Society Proc.* Vol. 99-11, May 1999, p289.
- Smith, S.; Mascarenhas, A.; Olson, J.M.; Kazmerski, L.L. "Spatially-resolved photoluminescence in spontaneously-ordered GaInP₂," *Materials Research Society conference proceedings (in press)*, November 1999.
- Dhere, R.G.; Cheong, H.; Smith, S.; Albin, D.S.; Mascarenhas, A.; Gessert, T. A. "Micro-PL Studies of Polycrystalline CdS/CdTe Interfaces," *Conf. Proc.*, NCPV Program Review, Denver, CO, April 16-19, 2000.

Presentations

- Mascarenhas, A.; Smith, S.; Cheong, H.M.; Fluegel, B.D.; Geisz, J.F.; Olson, J.M.; Kazmerski, L.L. "Excitons and Recombination in Photovoltaic materials," *NCPV Program Review*, Denver, CO, Sept. 1998.
- Smith, S.; Cheong, H.M.; Fluegel, B.D.; Geisz, J.F.; Olson, J.M.; Kazmerski, L.L. "Spatially Resolved Photoluminescence in Partially ordered GaInP₂," *March Meeting of the American Physical Society*, Atlanta, GA, March 1999.
- Smith, S.; Cheong, H.M.; Fluegel, B.D.; Geisz, J.F.; Olson, J.M.; Kazmerski, L.L. "Spatially resolved low-temperature photoluminescence in GaInP₂," *Quantum Optoelectronics Meeting of the Optical Society of America*, Aspen, CO, April 1999.
- Mascarenhas, A.; Smith, S.; Cheong, H.M.; Fluegel, B. D.; Olson, J.M. "Recombination Dynamics at Defects in Ordered GaInP," *International Conference on Spectroscopy of Semiconductor Structures*, Stuttgart, Germany, July 1999.
- Kao, Y.H.; Kazmerski, L.; Lynn, K.G.; Mascarenhas, A. "Photovoltaics Characterization: An Overview," *Annual Meeting of the Electrochemical Society*, Seattle, WA, May 1999.
- Smith, S.; Mascarenhas, A.; Olson, J.M.; Kazmerski, L.L. "Spatially Resolved Photoluminescence in Spontaneously-ordered GaInP₂," *Fall meeting of the Materials Research Society*, Boston, MA, November 1999.
- Smith, S.; Geisz, J.F.; Olson, J.M.; Kazmerski, L.L.; Mascarenhas, A. "Optical spectroscopy of spontaneously-ordered GaInP₂ with sub-micron spatial resolution," *March Meeting of the American Physical Society*, Minneapolis, MN, March 2000.

Proposals / Follow-on Funding

Follow-on Funding

- \$270K of external funding from DOE Office of Science was awarded to a collaborative team between Oak Ridge National Laboratory, Vanderbilt University, and NREL to expand and continue this work.

Brent Nelson

Anisotropy in Hydrogenated Thin-film Silicon Materials

Award: \$289.5K (\$100K for FY 2000)

Period of Performance: 10/99 to 9/01

Project Number: 06520003

Status: In Process

Description: This research involves a creative approach, at the forefront of materials characterization science, which will offer important new insights into the structural and electronic properties of hydrogenated silicon thin film (TF-SiH) materials. With this project as a proving ground, NREL researchers will strengthen the characterization methodology for TF-SiH, and may be relevant to other thin-film semiconductors materials.

Objective: The objective of this research is to advance materials science by characterizing the bonding configurations in TF-SiH. By acquiring and optimizing new infrared spectroscopy techniques we will be able to correlate optical characteristics of TF-SiH with the structural and electronic properties of these films.

Articles/Papers/Publications

Papers

- Webb, J. "Anisotropy In Hydrogenated Silicon Thin Films." *Materials Research Society Spring 2000 Meeting Proceedings*, San Francisco, CA. To be published.

Presentations

- Webb, J. "Anisotropy In Hydrogenated Silicon Thin Films." *Materials Research Society Spring 2000 Meeting*, San Francisco, CA., April 26, 2000.

New or Enhanced Collaborations

- Enhanced collaborations between NREL's FTIR lab, NREL's a-Si team, and the University of North Carolina, specifically to use photoluminescence to detect the onset of microcrystalline growth.

Randy Ellingson

Surface and Interface Studies by Second-order Nonlinear Optical Spectroscopy

Award: \$300K (\$100K for FY 2000)

Period of Performance: 10/99 to 9/02

Project Number: 06590003

Status: In Process

Description: Surface reactions play a central role in most photoelectrochemical and photocatalytic reactions, as well as in the very important electrocatalytic reactions in fuel cells. By developing a surface-specific optical spectroscopy technique, NREL stands to gain a foundation in the understanding of non-linear optical surface-specific characterizations as well as gain specific knowledge of important charge-transfer reactions for renewable energy technologies.

Objective: The objective of this research is to develop a surface-specific second-order nonlinear optical spectroscopy technique.

Distributed and Hybrid Energy Systems

John Turner

Advanced Fuel Cell Research

Award: \$426K

Period of Performance: 3/1/99 to 3/1/01

Project Number: 06540091

Status: In Process

Description: Fuel cells, especially when powered with hydrogen derived from a renewable energy resource, may represent an ideal energy technology. It couples an inexhaustible energy source with a zero-emission conversion technology that gives off no net carbon dioxide. This project is linking an important renewable resource, bioethanol, with fuel cells (the zero-emission technology) to give NREL an approach for developing a renewable power package for many applications, including vehicles and modular, distributed generation of electricity.

Objective: The objective of this research is to define and establish a leading role for NREL in the basic science, design, development, and validation of the next generation of fuel cell systems.

New or Enhanced Collaborations

- Collaborated with Dan DuBois of NREL and Barton Smith of the University of Colorado, linking state-of-the-art theoretical modeling of electrocatalysis with combinatorial synthesis procedures to identify promising non-precious metal catalysts for alcohol oxidation.

Scott Ward

Monolithically Integrated PV Modules for Dish Solar Concentrator Systems

Award: \$80K

Period of Performance: 6/99 to 5/01

Project Number: 06520091

Status: In Process

Description: Think of making a 2-square-foot PV module that could generate 50,000 watts of electric power. In essence, the success of this project would accomplish that. Researchers are exploring the concept of connecting III-V multi-junction solar cells monolithically, in series on a non-conductive substrate to make mini-modules that can be used under high solar concentration. This could lead to a next-generation technology that combines solar thermal concentrator technology with high-efficiency PV technology to produce inexpensive electric power systems.

Objective: The objective of this research is to use recently developed processing techniques to design and fabricate mini-modules from the GaInP/GaAs tandem device structure developed by NREL's high-efficiency PV team for use under high flux provided by dish concentrator systems.

Bill Marion

New Capabilities for Worldwide Weather Data Sets

Award: \$116.2K

Period of Performance: 10/99 to 9/00

Project Number: 06560001

Status: In Process

Description: For most locations worldwide, analysts, engineers, and planners do not have the hourly weather data needed for input to computer programs that simulate the performance of buildings, grid-connected and stand-alone photovoltaic (PV) systems, solar thermal electric systems, PV/wind/diesel hybrid systems, and distributed generation systems. This research provides NREL with a new capability, unmatched by any other organization, for developing worldwide weather data sets. The capability to develop hourly data sets and their associated products enhances the Laboratory's ability to address the potential for technology deployment by providing the necessary weather data for performance and economic analyses of renewable energy systems for virtually anywhere in the world.

Objective: The objective of this research is to develop a new capability for developing multi-year data sets of hourly solar radiation and meteorological data for locations throughout the world. With this capability, users can size and evaluate the performance and economics of renewable energy systems thereby reducing the risk in the deployment of renewables and aiding in the selection of the best renewable technology for a specific location.

New or Enhanced Collaborations

- Collaborated with NREL's solar thermal group to develop a TMY (typical meteorological year — a "typical" year of hourly solar and meteorological values, which is designed to pro-

duce the expected climate of a location throughout a year) for Upington, South Africa for use in evaluating concentrating solar power for this region.

- Collaborated with Dr. Robert Turner from Science Applications International Corporation (SAIC), who provided useful information on possible sources of aerosol data that we might obtain to expand our existing information on global aerosol amounts.
- Ray George collaborated with NASA scientists, securing two additional sources of aerosol data.

Proposals / Follow-on funding

Proposals

- Daryl Myers submitted an unsolicited proposal to NASA for \$200K.
- Dave Renné and Liz Brady submitted a proposal to the United Nations Environmental Program for \$400K.

Energy Efficiency

James Tangler

Performance Verification of NREL's Advanced Airfoils for Cooling Tower Fan Blades

Award: \$78.2K

Period of Performance: 7/99 to 9/00

Project Number: 06500091

Status: In Process

Description: The researchers leading this project hypothesize that improved NREL-designed airfoils will reduce the power requirement for cooling tower fans by 2%-5% relative to current technology, thereby improving energy efficiency. A successful test of these improvements would strengthen NREL's existing core competency in advanced airfoil design.

Objective: The objective of this research is to verify the predicted performance of advanced airfoils for high-efficiency cooling fan blades.

Articles/Papers/Publications

Papers

- Tangler, J.L., et al., "Advanced Airfoils for Cooling Tower Fan Blades," *1999 Cooling Tower Institute Annual Conference*, New Orleans, LA, February 1999.

Intellectual Property (Patents, Records of Invention, etc.)

A patent is pending on the two cooling tower fan airfoils (S905 root airfoil and S904 tip airfoil), designed through this study.

Christopher Gaul
Combined Compressor Pump Advanced Prototype
Award: \$15K (\$12.5K in FY 2000)
Period of Performance: 5/1/00 to 10/31/00
Project Number: 06350001
Status: In Process

Description: Refrigeration and air conditioning consume 15% of U.S. electric power. This project will develop an advanced prototype of a combined refrigeration compressor and liquid refrigerant pump to lower the cost of energy-saving cooling designs. Lower cost leads to expanded use and lower national energy consumption. While the product is aimed at a niche market, even a small piece of a \$40 billion worldwide refrigeration and air conditioning market will have a substantial impact.

Objective: The objective of this project is to demonstrate the feasibility of producing a combined refrigeration compressor and liquid refrigerant pump inexpensively enough to be practical wherever it is technically desirable.

Energy Analysis

Sam Baldwin / Brandon Owens
A Technology-Policy Expert System
Award: \$500K
Period of Performance: 10/1/98 to 9/30/01
(re-scoped, re-authorized 3/99. Approved for
FY 2000 funding 11/99)
Project Number: 06009130
Status: In Process

Description: In the 1990s, the emergence of the Internet initiated a fundamental transformation in the way that energy analysis is conducted and communicated. Institutionally dispersed analysts are beginning to achieve unparalleled results through on-line collaborations with remote colleagues. Formerly unaided decision-makers are now becoming equipped with specialized knowledge and capability through the proliferation Internet-based analysis applications. And previously uninformed stakeholders are opening themselves to the wealth of possibilities offered by Internet-based information dissemination.

NREL has made a strong commitment to becoming a leader in the emerging field of Internet-based energy analysis, or e-Analysis, by funding the Technology-Policy Expert System. Once complete, the Technology-Policy Expert System will shape the national energy debate by providing interested stakeholders with the ability to evaluate the effectiveness of alternative renewable energy policies by employing the same analysis tools and techniques that are used by analysis experts at NREL. The objective of the Technology-Policy Expert System is to test the hypothesis that Internet-based energy analysis will fundamentally advance renewable energy and energy efficiency technology policy.

Objective: The objective of this project is to test the hypothesis that providing real-time, on-line mechanisms to test model assumptions will fundamentally advance the way policy analysis is performed by enabling policy analysts to interact with stakeholders in developing consensus on model assumptions, and ultimately on preferred policy options.

Appendices

Appendix A. NREL DDRD Policy

I. POLICY STATEMENT

NREL funds discretionary research to maintain its scientific and technical vitality, enhance its ability to address future DOE missions, foster creativity and stimulate exploration of forefront science and technology, and to serve as a proving ground for new and potentially high-value mission enhancing activities.

II. GENERAL RULES

A. Director's Discretionary Research and Development (DDRD) Program

1. NREL implements this policy through the DDRD Program. The Program enables the Laboratory director to approve for funding projects put forth by Laboratory staff which propose to explore and/or develop innovative or creative opportunities within mission areas assigned to the Laboratory, and enables NREL to maintain the ability to support new ideas, approaches, and concepts in executing the assigned missions.
2. NREL's DDRD Program is consistent with DOE's position on Laboratory-Directed Research and Development at multiprogram funded laboratories and is consistent with the DOE mission. NREL's DDRD Program is specifically aligned with DOE's Office of Energy Efficiency and Renewable Energy (EE) policy on DDRD.
3. DDRD Program goals are to:
 - a. Maintain the scientific and technical vitality of the Laboratory.
 - b. Enhance the Laboratory's long-term viability by strengthening existing core competencies and building new capabilities.
 - c. Enhance the Laboratory's ability to address future DOE missions.
 - d. Foster creativity and stimulate exploration of forefront science and technology.
 - e. Serve as a proving ground for new and potentially high-value mission enhancing activities.

B. DDRD Program Criteria

1. Projects advance research and development directed toward solving present scientific or technical problems, or are experiments and analysis directed toward determining the merit and utility of new ideas or concepts.

2. Projects are generally limited to \$500,000 and to a duration of no more than 3 years. Exceptions are approved only by the Laboratory director.
3. Subcontracts, including consulting agreements and individual task orders issued against established task ordering agreements, may be used as an integral part of DDRD projects to obtain expertise that is not available at the Laboratory and contributes to building core capabilities at the Laboratory. Subcontracts should be of a magnitude that they support rather than dominate the capability building at the Laboratory. Generally, DDRD subcontracting is directed toward obtaining normal materials, supplies, services, and testing. These specific subcontracts, consulting agreements, or individual task orders will be awarded in conjunction with an approved DDRD project. Funding for these specific subcontracts, consulting agreements, and individual task orders will not be commingled with other subcontract projects.
4. Individual project costs, including all allocable costs except general and administrative expenses, are accumulated in a separate expense pool as part of the Laboratory's indirect costs, and are allocated equitably to all operating costs of the Laboratory.

C. DDRD Program Funding

1. NREL may annually approve DDRD projects not to exceed 2% of the Laboratory's estimated total operating funds from appropriations. The specific ceiling for project approvals is negotiated annually with the DOE Golden Field Office (GO) in consultation with the assistant secretary for EE.
2. To be approved for funding, DDRD project proposals must specifically address one or more of the DDRD Program goals.
3. The DDRD Program is not to be used to:
 - a. Substitute for or increase funding for any tasks for which a specific limitation has been established by Congress or DOE, or for any specific tasks that are funded by DOE or other users of the Laboratory.
 - b. Fund projects that will require the addition of non-DDRD funds to accomplish the technical goals of the project.
 - c. Fund capital and construction design beyond the preliminary phase (e.g., conceptual design, Title I design work, or any similar or more advanced design effort) or to fund construction line-item projects, in whole or in part.
 - d. Fund general purpose equipment expenditures with the exception of acquisition of low-value general purpose equipment that is clearly required for the project and is not otherwise readily available from the Laboratory inventory.

4. DDRD costs are allocated to direct programs through an overhead rate negotiated annually with GO. This allocation method is consistent with NREL's accounting policy. Individual DDRD project costs are tracked against approved project totals to provide for effective cost control and project management.

D. DDRD Review.

All DDRD projects are reviewed periodically by executive management, and the DDRD Program is reported annually to DOE by NREL.

III. RESPONSIBILITIES

A. Director

1. Endorses and supports NREL's policy on DDRD.
2. Sets the strategic direction for the DDRD Program.
3. Approves and transmits an annual DDRD Program report to EE.
4. Delegates DDRD Program leadership, process management, and administration to the associate director for Planning and Program Integration.

B. Associate Director for Planning and Program Integration

1. Provides overall DDRD leadership and process management according to the DDRD policy through a designated process leader.
2. Annually negotiates the specific level of funding for the DDRD Program with GO as part of the Cost Proposal.
3. Administers the process for soliciting and reviewing DDRD proposals and tracking results.
4. In consultation with the director and other associate directors, approves the DDRD Program portfolio of projects for funding and periodically reviews Program results.
5. Prepares periodic summary reports on DDRD for executive management.
6. Prepares the annual DDRD Program report before October 31 of each year that includes a listing of funded projects, a listing of completed projects, a clear description of each funded project and its objectives, highlights of the overall Program, and a summary of major project or Program accomplishments. Submits the report to the director for review, approval, and transmittal to DOE.

C. Senior Managers

1. Report overall project management and project results from their centers or offices to the DDRD process leader in Planning and Program Integration.
2. Mentor project managers through their line management.
3. Report on DDRD projects for executive management review.

D. DDRD Project Managers

1. Develop and execute project plans.
2. Manage the projects and their costs according to the project plans and report results.

E. Finance Office Director (Controller)

1. Includes the annually negotiated DDRD Program funding level in the annual Cost Proposal negotiated with DOE.
2. Provides the financial system infrastructure which accumulates project costs by individual project, includes all allocable costs except general and administrative expenses, accumulates costs in a separate expense pool as part of the Laboratory's indirect costs, and allocates costs equitably to all in-house operating costs of the Laboratory.

F. Employees and Other Workers.

Comply with NREL's policy on DDRD.

IV. REFERENCES

DOE Policy for Director's Discretionary Research and Development at the National Renewable Energy Laboratory, December 15, 1998

Signed by:

Bob Garrett
Associate Director
03/09/99

Original signed document on file in the Quality and Assessment Office.

Appendix B. DOE DDRD Policy

The Office of Energy Efficiency and Renewable Energy Policy for Laboratory Director's Discretionary Research and Development Program

It is the policy of the Office of Energy Efficiency and Renewable Energy (EE) to support a Director's Discretionary Research and Development Program at the National Renewable Energy Laboratory (NREL). The policy is consistent with the Department's position on Laboratory Directed Research and Development at multi-program-funded laboratories and is consistent with the mission of the Department. Authority for this policy is contained in Public Law 95-39 Section 303.

NREL will establish a Director's Discretionary Research and Development Program to be funded by EE and by other entities directly funding work at the laboratory. This program may utilize up to 2% of the annual estimated funding from Appropriations, excluding funding specifically identified for capital equipment or for construction. The specific level of funding will be negotiated annually between NREL and the Golden Field Office (GO), in consultation with the Office of the Assistant Secretary.

This program is to enable the Director to approve for funding projects put forth by laboratory staff, which propose to explore and/or develop innovative or creative opportunities within mission areas assigned to the laboratory. Projects should advance research and development directed toward solving present scientific or technical problems; or should be experiments and analysis directed toward determining the merit and utility of new ideas or concepts. Projects should generally be small (up to \$500,000) and of a limited duration (up to 3 years). It is not anticipated that, excepting normal materials, supplies, services and testing, subcontracting will be needed to accomplish these projects. It is anticipated that this program will enable NREL to maintain the ability to support new ideas, approaches and concepts in executing the assigned missions.

In accordance with the Department's financial policy, project costs will be accumulated by individual project, will include all allocable costs except general and administrative expenses, will be accumulated in a separate expense pool as part of laboratories' indirect costs, and will be allocated equitably to all operating costs of the laboratory.

The Director will provide an annual report to the Department of this program that will include a listing of funded projects, a listing of completed projects, a clear description of each funded project and its objectives, highlights of the overall program and a summary of major project or program accomplishments. This report will be due October 31st of each year.

The Assistant Secretary for Energy Efficiency and Renewable Energy with the participation of GO and other EE representatives will conduct an annual review of the program to coincide with the submission of the annual report. This policy is effective December 1, 1998.

Signed by Dan Reicher, Assistant Secretary for Energy Efficiency and Renewable Energy,
December 15, 1998.

Appendix C. DDRD Proposal Template

Director's Discretionary Research and Development (DDRD) Program Proposal Template

ALL SECTIONS OF THE TEMPLATE MUST BE COMPLETED FOR THE PROPOSAL TO BE ACCEPTED FOR CONSIDERATION.

PI Name: _____
(The PI must be an NREL Employee, and not a Post Doc)

PI Phone: _____

PI Fax: _____

PI Location: _____

PI Email: _____

Proposal Title: _____

Expected Outcome: _____

Requested Funding (total and by year): _____

Requested Funding Period: _____

Team Members: _____; _____;

The NREL mission is

To lead the nation toward a sustainable energy future by developing renewable energy technologies, improving energy efficiency, advancing related science and engineering, and facilitating deployment.

How does the proposed project contribute to mission success?

Projects should advance research and development directed toward solving present scientific technical problems, or should be experiments and analysis directed toward determining the merit and utility of new ideas and concepts.

How does the proposed project address one or both of these overarching goals?

The goals of the DDRD Program are to:

- **Maintain scientific and technical vitality of the Laboratory**
- **Enhance the Laboratory's long-term viability by strengthening existing core competencies and building new capabilities**
- **Enhance the Laboratory's ability to address future DOE missions**
- **Foster creativity and stimulate exploration of forefront science and technology**
- **Serve as a proving ground for new and potentially high-value mission enhancing activities**

How does the proposed project specifically address one or more of these program goals?

DDRD funds are not to be used to:

- **substitute for or increase funding for any tasks for which a specific limitation has been established by Congress or DOE, or for any specific tasks that are funded by DOE or other users of the Laboratory.**
- **Fund projects that will require the addition of non-DDRD funds to accomplish the technical goals of the project.**
- **Fund design beyond the preliminary phase (e.g., conceptual design, Title I design work, or any similar or more advanced design effort) or to fund construction line-item projects, in whole or in part.**
- **Fund general purpose capital expenditures with the exception of acquisition of general purpose equipment that is clearly required for the project and is not otherwise readily available from the Laboratory inventory.**

Does the proposed project meet these criteria? What is the relationship of this work to current programs?

The proposed project can be proposed for up to \$500,000 in funding and for a duration of up to three years. (If there are several projects proposed under a strategic initiative, each project must be proposed separately using this template and must be no more than \$500,000 each)

Does the proposed project meet this criterion?

Subcontracts, including consulting agreements and individual task orders issued against established task ordering agreements (TOAs), and post docs may be used as an integral part of the DDRD projects to obtain expertise that (1) is not available at the Laboratory and (2) contributes to building core capabilities at the Laboratory. Subcontracts should be of a magnitude that they support rather than dominate the capability-building at the Laboratory. Generally, subcontracting is directed toward obtaining normal materials, supplies, services, and testing. These specific subcontracts, consulting agreements, or individual task orders will be awarded in conjunction with an approved DDRD project. Funding for these specific subcontracts, consulting agreements, and individual task orders will not be commingled with other subcontract projects.

Does the proposed project meet this criterion? What outside work is planned? Who are the subcontractors and what is the dollar amount for each?

List the titles for all proposals (funded or not) submitted under NREL's discretionary R&D program (DDF, FIRST, or DDRD) during the past 5 years in which you were the principal investigator or one of the investigators. Please also briefly describe the relationship, if any, between the proposal you are currently submitting and work supported previously or presently by DOE Programs.

Are you aware of any on-going research at NREL that is similar to what you are proposing? To your knowledge, has the research you are proposing been proposed elsewhere at the Laboratory?

Provide information under each of the following topics:

- Abstract/Concept – statement of the research problem or need (1/2 page)
- Background (1 page)
- Approach (2 pages)
- Measure of Successful Outcome (1 page)
- Intellectual Property and Patent Considerations (including any background intellectual property (ROIs) or patent and patent applications or copyrights that are necessary to perform the work envisioned under this proposal) (1/2 page)
- Project Management
 - Performance Period
 - Staffing (Name, Role, Organization, Phone, FTE months)
- Cost
 - Loaded Labor
 - Other Direct Costs
 - Subcontracts (if any)
- Milestones
 - Milestones and Dates

Center / Office Director's Signature (required on all proposals). Center / Office Director signature means:

- Endorsement of the proposal *for going forward for consideration* in the DDRD review and approval process.
- Appropriate forethought has been given to managing Center / Office resources (staffing, facilities such as office and lab space, equipment such as computers, etc.) should the DDRD proposal be funded.
- Appropriate communications have taken place between Center / Office Directors and group managers, team leaders, and task leaders regarding managing the Center / Office resources and meeting existing milestones should the DDRD proposal be funded.
- The proposal complies with NREL Policies and Procedures, such as not augmenting program funding.
- The proposal does not duplicate on-going, funded research at the Laboratory.

Center / Office Director Signature

Center / Office Director (print name)